stochastic perturbation theory

a prequel to Reptation Quantum Monte Carlo

Stefano Baroni
Scuola Internazionale Superiore di Studi Avanzati
Trieste — Italy

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disclaimer

variational Quantum Monte Carlo

the Langevin way:

$$E_0 \lesssim \langle \Phi_0 | \hat{H} | \Phi_0 \rangle$$
$$= \int \Phi_0(R) \hat{H} \Phi_0(R) dR$$

where:

$$\hat{H} = -\frac{\partial^2}{\partial R^2} + V(R),$$
$$R = \{r_1, r_2, \cdots, r_N\}$$

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$$\approx \frac{1}{T} \int_0^T \mathcal{W}\big(R(t)\big) dt,$$

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$$\langle dW_t^2 \rangle = 2dt$$
$$\mathcal{F}(R) = -\frac{\partial \mathcal{U}(R)}{\partial R}$$
$$\mathcal{U}(R) = -\log\big(\Phi_0(R)^2\big)$$
$$\mathcal{F}(R) = 2\frac{1}{\Phi_0} \frac{\partial \Phi_0}{\partial X}$$

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estimating the statistical error:

$$\Delta E_T^2 \approx \frac{1}{T^2} \left\langle \left[\int_0^T \Big(\mathcal{W}\big(R(t)\big) - \langle \mathcal{W} \rangle \Big) dt \right]^2 \right\rangle$$

variational Quantum Monte Carlo

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variational Quantum Monte Carlo

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$$\doteq \frac{2\tau_{\mathcal{W}}}{T} \Delta \mathcal{W}^2$$

Langevin dynamics

$$dR = \mathcal{F}(R)dt + dW_t$$

$$\langle dW_t^2 \rangle = 2dt$$

$$\mathcal{F}(R) = -\frac{\partial \mathcal{U}(R)}{\partial R}$$

$$\frac{\partial P(R,t)}{\partial t} = \frac{\partial^2 P(R,t)}{\partial R^2} - \frac{\partial}{\partial R}\big(\mathcal{F}(R)P(R,t)\big)$$

$$P_0(R) \propto \mathrm{e}^{-\mathcal{U}(R)}$$

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$$\mathcal{V}(R) = \frac{1}{4}\mathcal{F}(R)^2 - \frac{1}{2}\Delta\mathcal{U}(R)$$

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$$\Phi(R,t) = P(R,t)/\Phi_0(R)$$

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$$\hat{\mathcal{H}}\Phi_0 = 0$$
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$$\begin{aligned} P(R,t) &= \int W(R,t|R',0)P(R',0)dR' \\ &= \Phi_0(R)\Phi(R,t) \\ &= \Phi_0(R)\int \underbrace{\mathcal{G}(R,t;R',0)}_{\langle R|\mathrm{e}^{-\hat{\mathcal{H}}(t-t')}|R'\rangle} \Phi(R',0)dR' \end{aligned}$$

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$$W(R,t|R',0) = \Phi_0(R)\mathcal{G}(R,t;R',0)/\Phi_0(R')$$

computing the local-energy correlation time

summary:

$$dR = \mathcal{F}(R)dR + dW_t$$

$$\frac{\partial P(R,t)}{\partial t} = \frac{\partial^2 P(R,t)}{\partial R^2} - \frac{\partial}{\partial R}(\mathcal{F}(R)P(R,t))$$

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$$\langle \Delta\mathcal{W}(t)\Delta\mathcal{W}(0)\rangle = \int \Delta\mathcal{W}(R)\Delta\mathcal{W}(R')P(R,t;R',0)dRdR'$$

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$$\begin{aligned}\tau_{\mathcal{W}}\Delta\mathcal{W}^2 &\doteq \int_0^\infty \langle \Phi_0|\Delta\widehat{\mathcal{W}}\widehat{\mathcal{G}}(t)\Delta\widehat{\mathcal{W}}|\Phi_0\rangle dt \\ &= \sum_{n>0}\frac{|\mathcal{W}_{0n}|2}{\mathcal{E}_n}\end{aligned}$$

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$$\tau_{\mathcal{W}} = \frac{1}{\Delta\mathcal{W}^2}\sum_{n>0}\frac{|\mathcal{W}_{0n}|2}{\mathcal{E}_n}$$

second-order perturbation theory

$$\widehat{H} = \widehat{\mathcal{H}} + \mathcal{W}(R)$$

$$\begin{aligned}\tau_{\mathcal{W}} &= \frac{1}{\Delta\mathcal{W}^2} \sum_{n>0} \frac{|\mathcal{W}_{0n}|2}{\mathcal{E}_n} \\ &= -\frac{E_0^{(2)}}{\Delta\mathcal{W}^2}\end{aligned}$$

$$\begin{aligned}E_0 &= \cancel{\mathcal{E}_0} + \langle \Phi_0 | \widehat{\mathcal{W}} | \Phi_0 \rangle_{QM} - \sum_{n>0} \frac{|\langle \Phi_0 | \widehat{\mathcal{W}} | \Phi_n \rangle_{QM}|^2}{\cancel{\Delta}\mathcal{E}_n} + \cdots \\ &\sim \frac{d}{dT}\left[\underbrace{\left\langle \int_0^T \mathcal{W}(t)dt \right\rangle_{RW}}_{\mu_1[\mathcal{W}]} - \frac{1}{2} \underbrace{\left\langle \left(\int_0^T \Delta\mathcal{W}(t)dt \right)^2 \right\rangle_{RW}}_{\bar{\mu}_2[\mathcal{W}]} + \cdots ? \cdots \right]\end{aligned}$$

higher-order perturbation theory

$$\widehat{H} = \widehat{\mathcal{H}} + \mathcal{W}(R)$$

$$\Phi_0 = c_0 \Psi_0 + c_1 \Psi_1 + \cdots$$

$$\langle \Phi_0 | \mathrm{e}^{-\widehat{H} T} | \Phi_0 \rangle = c_0^2 \mathrm{e}^{-E_0 T} + c_1^2 \mathrm{e}^{-E_1 T} + \cdots$$

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$$\log\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle = -E_0T + \log\left(c_0^2 + c_1^2\mathrm{e}^{-\Delta E_1T} + \cdots\right)$$

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$$E_0 = -\frac{d}{dT}\log\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle + \mathcal{O}\left(e^{-\Delta E_1T}\right)$$

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higher-order perturbation theory

$$\widehat{H} = \widehat{\mathcal{H}} + \mathcal{W}(R)$$

$$E_0 = -\frac{d}{dT}\log\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle$$

$$\mathrm{e}^{-\hat{H}T} = \mathrm{e}^{-\hat{\mathcal{H}}T}\Bigg(1 - \int_0^T dt_1 \widehat{\mathcal{W}}(t_1)dt_1 + \int_0^T dt_2 \widehat{\mathcal{W}}(t_2)\int_0^{t_2} \widehat{\mathcal{W}}(t_1)dt_1 +$$

$$\cdots \frac{(-)^n}{n!}\int_{0\cdots 0}^{T\cdots T}\!\!\cdots\int \mathcal{T}\left(\widehat{\mathcal{W}}(t_1)\cdots\widehat{\mathcal{W}}(t_n)\right)dt_1\cdots dt_n + \cdots\Bigg)$$

higher-order perturbation theory

$$\widehat{H} = \widehat{\mathcal{H}} + \mathcal{W}(R)$$

$$E_0 = -\frac{d}{dT} \log \langle \Phi_0 | e^{-\widehat{H}T} | \Phi_0 \rangle$$

$$e^{-\hat{H}T} = e^{-\hat{\mathcal{H}}T} \Bigg(1 - \int_0^T dt_1 \widehat{\mathcal{W}}(t_1) dt_1 + \int_0^T dt_2 \widehat{\mathcal{W}}(t_2) \int_0^{t_2} \widehat{\mathcal{W}}(t_1) dt_1 + \cdots \frac{(-)^n}{n!} \int_{0\cdots0}^{T\cdots T} \cdots \int \mathcal{T} \left(\widehat{\mathcal{W}}(t_1) \cdots \widehat{\mathcal{W}}(t_n) \right) dt_1 \cdots dt_n + \cdots \Bigg)$$

$$\widehat{\mathcal{W}}(t) \doteq e^{\widehat{\mathcal{H}}t} \widehat{\mathcal{W}} e^{-\widehat{\mathcal{H}}t}$$

higher-order perturbation theory

$$\widehat{H} = \widehat{\mathcal{H}} + \mathcal{W}(R)$$

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$$\left. \cdots\frac{(-)^n}{n!}\int_{0\cdots 0}^{T\cdots T}\cdots\int\mathcal{T}\left(\widehat{\mathcal{W}}(t_1)\cdots\widehat{\mathcal{W}}(t_n)\right)dt_1\cdots dt_n + \cdots\right)$$

$$\widehat{\mathcal{W}}(t) \doteq e^{\widehat{\mathcal{H}}t}\,\widehat{\mathcal{W}}\,e^{-\widehat{\mathcal{H}}t}$$

$$\langle\Phi_0|e^{-\widehat{H}T}|\Phi_0\rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots\frac{(-)^n}{n!}\mu_n + \cdots$$

$$\mu_n = n!\int_0^T dt_n\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_2}dt_1\langle\Phi_0|\widehat{\mathcal{W}}(t_n)\widehat{\mathcal{W}}(t_{n-1})\cdots\widehat{\mathcal{W}}(t_1)|\Phi_0\rangle_{QM}$$

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$$\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots$$

$$\mu_n = n! \int_0^T dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \langle\Phi_0|\widehat{\mathcal{W}}(t_n)\widehat{\mathcal{W}}(t_{n-1})\cdots\widehat{\mathcal{W}}(t_1)|\Phi_0\rangle_{QM}$$

$$\langle\Phi_0|\widehat{\mathcal{W}}(t_n)\widehat{\mathcal{W}}(t_{n-1})\cdots\widehat{\mathcal{W}}(t_1)|\Phi_0\rangle_{QM} = \int \Phi_0(R_n)\mathcal{W}(R_n)\mathcal{G}(R_n, t_n, R_{n-1}, t_{n-1}) \times \cdots \mathcal{W}(R_1)\mathcal{G}(R_2, t_2; R_2, t_1)\mathcal{W}(R_1)\Phi_0(R_1)\ dR_n \cdots dR_1$$

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higher-order perturbation theory

$$\langle \Phi_0 | \mathrm{e}^{-\widehat{H}T} | \Phi_0 \rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots$$

$$\mu_n = n! \int_0^T dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \langle \Phi_0 | \widehat{\mathcal{W}}(t_n) \widehat{\mathcal{W}}(t_{n-1}) \cdots \widehat{\mathcal{W}}(t_1) | \Phi_0 \rangle_{QM}$$

$$\begin{aligned} \langle \Phi_0 | \widehat{\mathcal{W}}(t_n) \widehat{\mathcal{W}}(t_{n-1}) \cdots \widehat{\mathcal{W}}(t_1) | \Phi_0 \rangle_{QM} &= \int \Phi_0(R_n) \mathcal{W}(R_n) \mathcal{G}(R_n, t_n, R_{n-1}, t_{n-1}) \\ &\quad \times \cdots \mathcal{W}(R_1) \mathcal{G}(R_2, t_2; R_2, t_1) \mathcal{W}(R_1) \Phi_0(R_1)\ dR_n \cdots dR_1 \\ &= \int W(R_n, t_n | R_{n-1}, t_{n-1}) \cdots W(R_2, t_2 | R_1, t_1) P_0(R_1) \\ &\quad \times \mathcal{W}(R_n) \cdots \mathcal{W}(R_1)\ dR_n \cdots dR_1 \end{aligned}$$

higher-order perturbation theory

$$\langle \Phi_0 | \mathrm{e}^{-\widehat{H}T} | \Phi_0 \rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots$$

$$\mu_n = n! \int_0^T dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \langle \Phi_0 | \widehat{\mathcal{W}}(t_n) \widehat{\mathcal{W}}(t_{n-1}) \cdots \widehat{\mathcal{W}}(t_1) | \Phi_0 \rangle_{QM}$$

$$\begin{aligned}
\langle \Phi_0 | \widehat{\mathcal{W}}(t_n) \widehat{\mathcal{W}}(t_{n-1}) \cdots \widehat{\mathcal{W}}(t_1) | \Phi_0 \rangle_{QM} &= \int \Phi_0(R_n) \mathcal{W}(R_n) \mathcal{G}(R_n, t_n, R_{n-1}, t_{n-1}) \\
&\quad \times \cdots \mathcal{W}(R_1) \mathcal{G}(R_2, t_2; R_2, t_1) \mathcal{W}(R_1) \Phi_0(R_1) \; dR_n \cdots dR_1 \\
&= \int W(R_n, t_n | R_{n-1}, t_{n-1}) \cdots W(R_2, t_2 | R_1, t_1) P_0(R_1) \\
&\qquad \times \mathcal{W}(R_n) \cdots \mathcal{W}(R_1) \; dR_n \cdots dR_1 \\
&\doteq \langle \mathcal{W}(t_n) \mathcal{W}(t_{n-1}) \cdots \mathcal{W}(t_1) \rangle_{RW}
\end{aligned}$$

higher-order perturbation theory

$$\langle \Phi_0 | \mathrm{e}^{-\widehat{H}T} | \Phi_0 \rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots$$

$$\mu_n = n! \int_0^T dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \langle \Phi_0 | \widehat{\mathcal{W}}(t_n) \widehat{\mathcal{W}}(t_{n-1}) \cdots \widehat{\mathcal{W}}(t_1) | \Phi_0 \rangle_{QM}$$

$$= \left\langle \left[\int_0^T \mathcal{W}(t) dt \right]^n \right\rangle_{RW}$$

$$\langle \Phi_0 | \widehat{\mathcal{W}}(t_n) \widehat{\mathcal{W}}(t_{n-1}) \cdots \widehat{\mathcal{W}}(t_1) | \Phi_0 \rangle_{QM} = \int \Phi_0(R_n) \mathcal{W}(R_n) \mathcal{G}(R_n, t_n, R_{n-1}, t_{n-1})$$

$$\times \cdots \mathcal{W}(R_1) \mathcal{G}(R_2, t_2; R_2, t_1) \mathcal{W}(R_1) \Phi_0(R_1) \; dR_n \cdots dR_1$$

$$= \int W(R_n, t_n | R_{n-1}, t_{n-1}) \cdots W(R_2, t_2 | R_1, t_1) P_0(R_1)$$

$$\times \mathcal{W}(R_n) \cdots \mathcal{W}(R_1) \; dR_n \cdots dR_1$$

$$\doteq \langle \mathcal{W}(t_n) \mathcal{W}(t_{n-1}) \cdots \mathcal{W}(t_1) \rangle_{RW}$$

infinite-order perturbation theory

$$\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots$$

$$\mu_n = \left\langle \left[\int_0^T \mathcal{W}(t)dt\right]^n \right\rangle_{RW}$$

infinite-order perturbation theory

$$\langle\Phi_0|e^{-\widehat{H}T}|\Phi_0\rangle_{QM} = 1-\mu_1+\frac{1}{2}\mu_2+\cdots\frac{(-)^n}{n!}\mu_n+\cdots$$
$$= \left\langle e^{-\int_0^T \mathcal{W}(t)dt}\right\rangle_{RW}$$
$$\doteq \left\langle e^{-\mathcal{S}(T)}\right\rangle_{RW}$$

$$\mu_n = \left\langle \left[\int_0^T \mathcal{W}(t)dt\right]^n \right\rangle_{RW}$$

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infinite-order perturbation theory

$$
\begin{aligned}
\langle \Phi_0 | \mathrm{e}^{-\widehat{H}T} | \Phi_0 \rangle_{QM} &= 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots \\
&= \left\langle \mathrm{e}^{-\int_0^T \mathcal{W}(t)dt} \right\rangle_{RW} \\
&\doteq \left\langle \mathrm{e}^{-\mathcal{S}(T)} \right\rangle_{RW}
\end{aligned}
$$

$$
\mu_n = \left\langle \left[\int_0^T \mathcal{W}(t)dt \right]^n \right\rangle_{RW}
$$

$$
E_0 \sim \frac{d}{dT} \log \langle \Phi_0 | \mathrm{e}^{-\widehat{H}T} | \Phi_0 \rangle_{QM}
$$

infinite-order perturbation theory

$$\langle \Phi_0 | e^{-\widehat{H}T} | \Phi_0 \rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots$$
$$= \left\langle e^{-\int_0^T \mathcal{W}(t)dt} \right\rangle_{RW}$$
$$\doteq \left\langle e^{-\mathcal{S}(T)} \right\rangle_{RW}$$

$$\mu_n = \left\langle \left[\int_0^T \mathcal{W}(t)dt \right]^n \right\rangle_{RW}$$

$$E_0 \sim \frac{d}{dT} \log \langle \Phi_0 | e^{-\widehat{H}T} | \Phi_0 \rangle_{QM}$$
$$= \frac{\left\langle \mathcal{W}(T) e^{-\mathcal{S}(T)} \right\rangle_{RW}}{\left\langle e^{-\mathcal{S}(T)} \right\rangle_{RW}}$$

infinite-order perturbation theory

$$\begin{aligned}\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle_{QM} &= 1-\mu_1+\frac{1}{2}\mu_2+\cdots\frac{(-)^n}{n!}\mu_n+\cdots\\ &= \left\langle \mathrm{e}^{-\int_0^T \mathcal{W}(t)dt}\right\rangle_{RW}\\ &\doteq \left\langle \mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}\end{aligned}$$

$$\mu_n = \left\langle\left[\int_0^T \mathcal{W}(t)dt\right]^n\right\rangle_{RW}$$

$$\begin{aligned}E_0 &\sim \frac{d}{dT}\log\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle_{QM}\\ &= \frac{\left\langle\mathcal{W}(T)\mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}{\left\langle\mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}\\ &= \frac{\left\langle\frac{\mathcal{S}(T)}{T}\mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}{\left\langle\mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}\end{aligned}$$

infinite-order perturbation theory

$$\langle\Phi_0|e^{-\widehat{H}T}|\Phi_0\rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots$$
$$= \left\langle e^{-\int_0^T \mathcal{W}(t)dt} \right\rangle_{RW}$$
$$\doteq \left\langle e^{-\mathcal{S}(T)} \right\rangle_{RW}$$

$$\mu_n = \left\langle \left[\int_0^T \mathcal{W}(t)dt\right]^n \right\rangle_{RW}$$

$$\widehat{H}(\boldsymbol{\lambda}) = \widehat{H} + \sum_i \lambda_i \widehat{A}_i$$

$$E_0 \sim \frac{d}{dT}\log\langle\Phi_0|e^{-\widehat{H}T}|\Phi_0\rangle_{QM}$$
$$= \frac{\left\langle \mathcal{W}(T)e^{-\mathcal{S}(T)} \right\rangle_{RW}}{\left\langle e^{-\mathcal{S}(T)} \right\rangle_{RW}}$$
$$= \frac{\left\langle \frac{\mathcal{S}(T)}{T} e^{-\mathcal{S}(T)} \right\rangle_{RW}}{\left\langle e^{-\mathcal{S}(T)} \right\rangle_{RW}}$$

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infinite-order perturbation theory

$$\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle_{QM} = 1-\mu_1+\frac{1}{2}\mu_2+\cdots\frac{(-)^n}{n!}\mu_n+\cdots$$
$$= \left\langle \mathrm{e}^{-\int_0^T \mathcal{W}(t)dt}\right\rangle_{RW}$$
$$\doteq \left\langle \mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}$$

$$\mu_n = \left\langle \left[\int_0^T \mathcal{W}(t)dt\right]^n \right\rangle_{RW}$$

$$\widehat{H}(\boldsymbol{\lambda}) = \widehat{H} + \sum_i \lambda_i \widehat{A}_i$$

$$E_0 \sim \frac{d}{dT}\log\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle_{QM}$$
$$= \frac{\left\langle \mathcal{W}(T)\mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}{\left\langle \mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}$$
$$= \frac{\left\langle \frac{\mathcal{S}(T)}{T}\mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}{\left\langle \mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}$$

$$\langle\widehat{A}_i\rangle = \left.\frac{\partial E_0(\boldsymbol{\lambda})}{\partial\lambda_i}\right|_{\boldsymbol{\lambda}=0}$$
$$= \frac{\left\langle \mathrm{e}^{-\mathcal{S}(T)}\frac{1}{T}\int_0^T \mathcal{A}(t)dt\right\rangle_{RW}}{\left\langle \mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}} \doteq \left\langle\!\!\left\langle \frac{1}{T}\int_0^T \mathcal{A}(t)dt \right\rangle\!\!\right\rangle$$

infinite-order perturbation theory

$$\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle_{QM} = 1-\mu_1+\frac{1}{2}\mu_2+\cdots\frac{(-)^n}{n!}\mu_n+\cdots$$
$$= \left\langle \mathrm{e}^{-\int_0^T \mathcal{W}(t)dt}\right\rangle_{RW}$$
$$\doteq \left\langle \mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}$$

$$\mu_n = \left\langle \left[\int_0^T \mathcal{W}(t)dt\right]^n\right\rangle_{RW}$$

$$\widehat{H}(\boldsymbol{\lambda}) = \widehat{H}+\sum_i \lambda_i \widehat{A}_i$$

$$E_0 \sim \frac{d}{dT}\log\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle_{QM}$$
$$= \frac{\left\langle \mathcal{W}(T)\mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}{\left\langle \mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}$$
$$= \frac{\left\langle \frac{\mathcal{S}(T)}{T}\mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}{\left\langle \mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}}$$

$$\langle\widehat{A}_i\rangle = \left.\frac{\partial E_0(\boldsymbol{\lambda})}{\partial\lambda_i}\right|_{\boldsymbol{\lambda}=0}$$
$$= \frac{\left\langle \mathrm{e}^{-\mathcal{S}(T)}\frac{1}{T}\int_0^T\mathcal{A}(t)dt\right\rangle_{RW}}{\left\langle \mathrm{e}^{-\mathcal{S}(T)}\right\rangle_{RW}} \doteq \left\langle\!\!\left\langle \frac{1}{T}\int_0^T \mathcal{A}(t)dt\right\rangle\!\!\right\rangle$$

$$\frac{\partial\langle\widehat{A}_i\rangle}{\partial\lambda_j} = 2\int_0^T C_{ij}(t)dt$$
$$C_{ij}(t) = \langle\!\langle \Delta\mathcal{A}_i(t)\Delta\mathcal{A}_j(0)\rangle\!\rangle$$
$$= \langle\Delta\widehat{A}_i(-it)\Delta\widehat{A}_j(0)\rangle_{QM}$$

Reptation Quantum Monte Carlo

$$\langle \widehat{A} \rangle \sim \left\langle e^{-\mathcal{S}} \frac{1}{T} \int_0^T \mathcal{A}(t) dt \right\rangle_{RW}$$

$$\langle \Phi_0 | e^{-\widehat{H}T} | \Phi_0 \rangle \sim \left\langle e^{-\int_0^T \mathcal{E}(t) dt} \right\rangle_{RW}$$

$$\langle A(-it) A(0) \rangle = \left\langle e^{-\mathcal{S}} \frac{1}{T} \int_0^T A(t' + t) A(t') dt \right\rangle_{RW}$$

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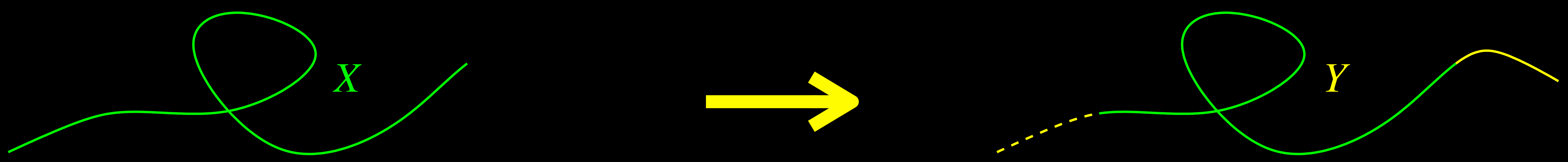
Reptation Quantum Monte Carlo

$$\langle \widehat{A} \rangle \sim \left\langle \mathrm{e}^{-\mathcal{S}} \frac{1}{T}\int_0^T \mathcal{A}(t)dt \right\rangle_{RW}$$

$$\langle \Phi_0 | \mathrm{e}^{-\widehat{H}T} | \Phi_0\rangle \sim \left\langle \mathrm{e}^{-\int_0^T \mathcal{E}(t)dt}\right\rangle_{RW}$$

$$\langle A(-it)A(0)\rangle = \left\langle \mathrm{e}^{-\mathcal{S}} \frac{1}{T}\int_0^T A(t'+t)A(t')dt\right\rangle_{RW}$$

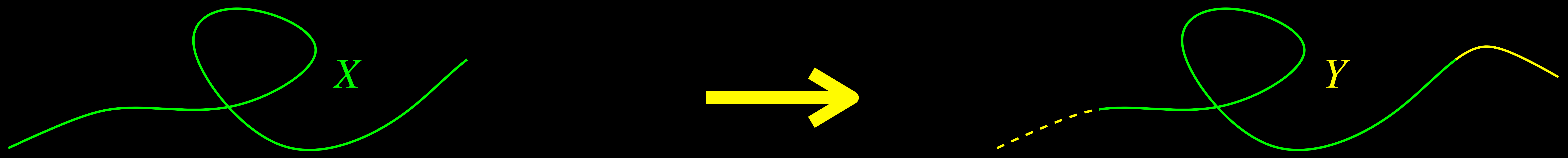


Reptation Quantum Monte Carlo

$$\langle \widehat{A} \rangle \sim \left\langle e^{-\mathcal{S}} \frac{1}{T} \int_0^T \mathcal{A}(t) dt \right\rangle_{RW}$$

$$\langle \Phi_0 | e^{-\widehat{H}T} | \Phi_0 \rangle \sim \left\langle e^{-\int_0^T \mathcal{E}(t) dt} \right\rangle_{RW}$$

$$\langle A(-it) A(0) \rangle = \left\langle e^{-\mathcal{S}} \frac{1}{T} \int_0^T A(t'+t) A(t') dt \right\rangle_{RW}$$



$$\texttt{accept}[X \to Y] = \min\left(1, e^{-\Delta \mathcal{S}}\right)$$

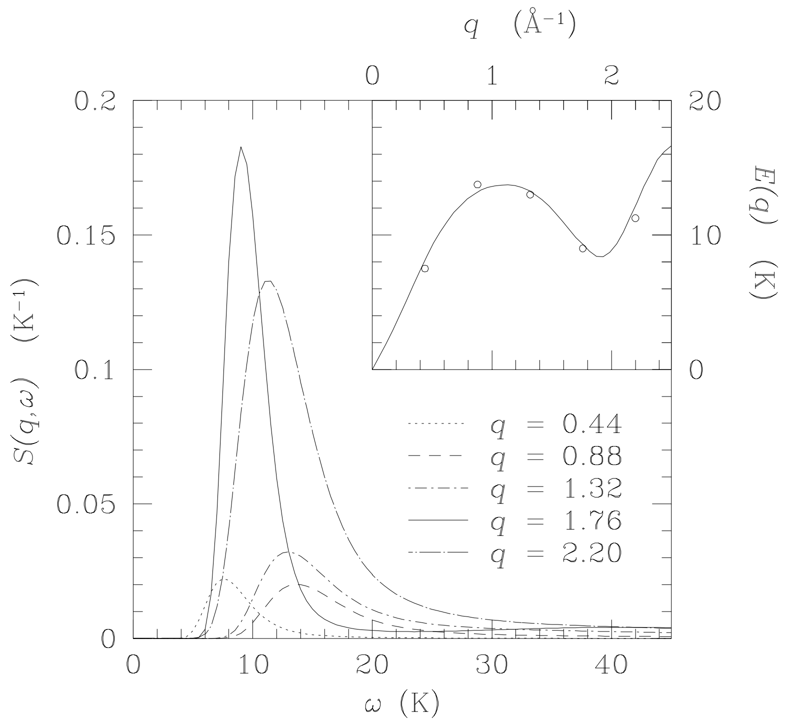
a few highlights

REPTATION QUANTUM MONTE CARLO

a round-trip tour from classical diffusion to quantum mechanics

STEFANO BARONI* AND SAVERIO MORONI†

Proceedings of the NATO ASI Quantum Monte Carlo Methods in Physics and Chemistry, Cornell University, July, 12-25, 1998



a few highlights

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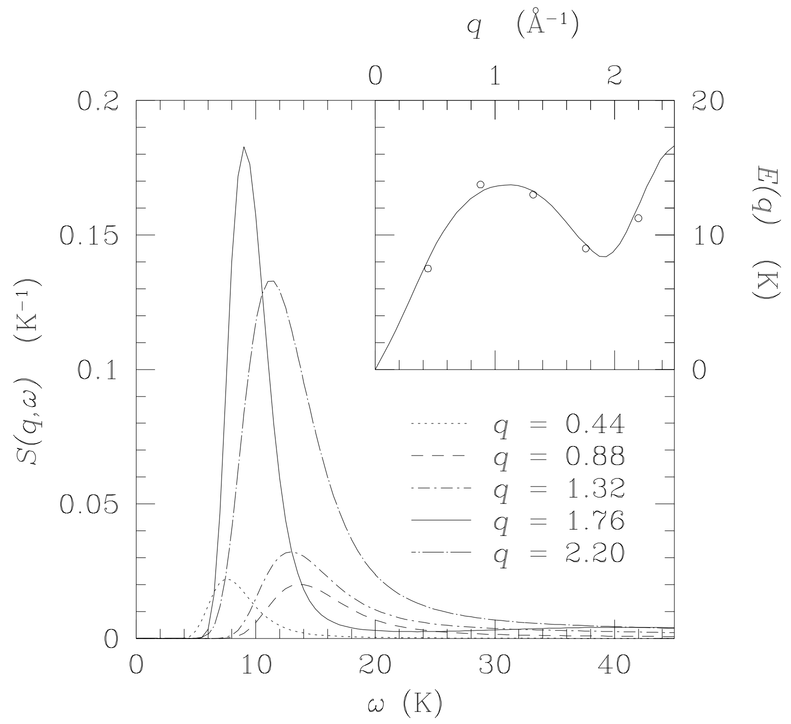
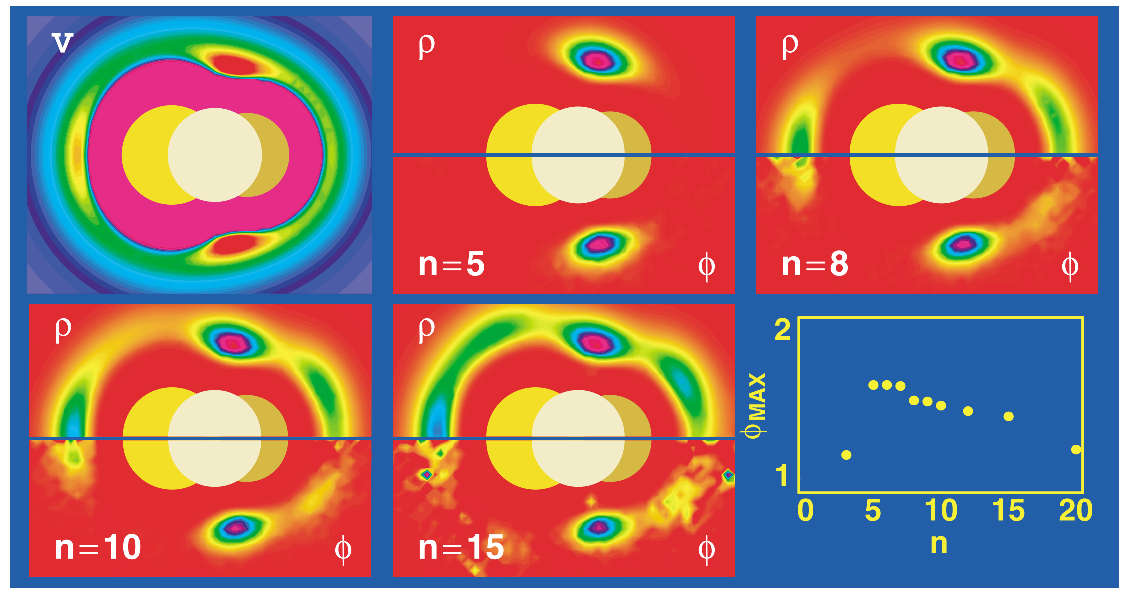


VOLUME 90, NUMBER 14 PHYSICAL REVIEW LETTERS week ending 11 APRIL 2003

Structure, Rotational Dynamics, and Superfluidity of Small OCS-Doped He Clusters

Saverio Moroni,[1] Antonio Sarsa,[2,*] Stefano Fantoni,[2] Kevin E. Schmidt,[2,†] and Stefano Baroni[2,3,‡]



a few highlights

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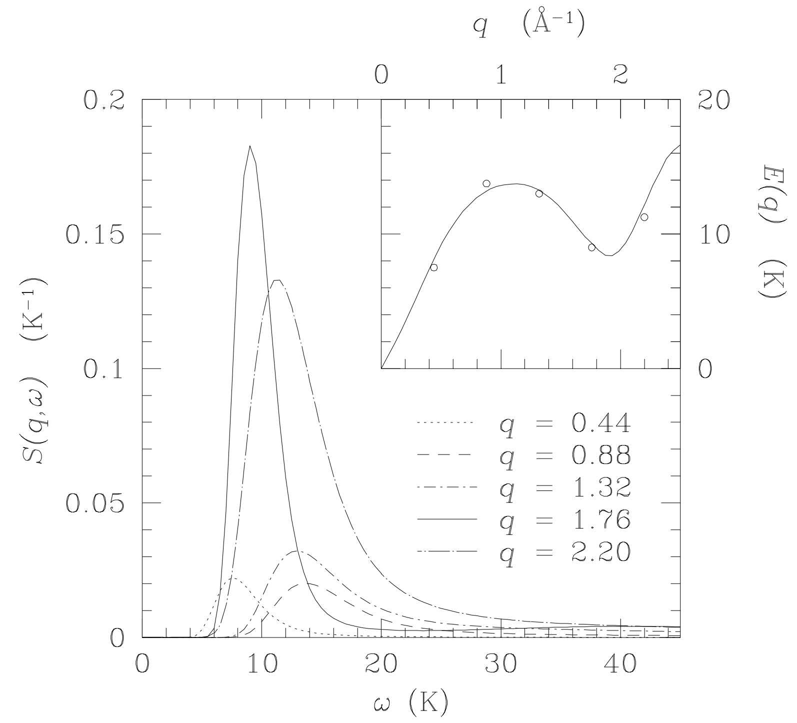

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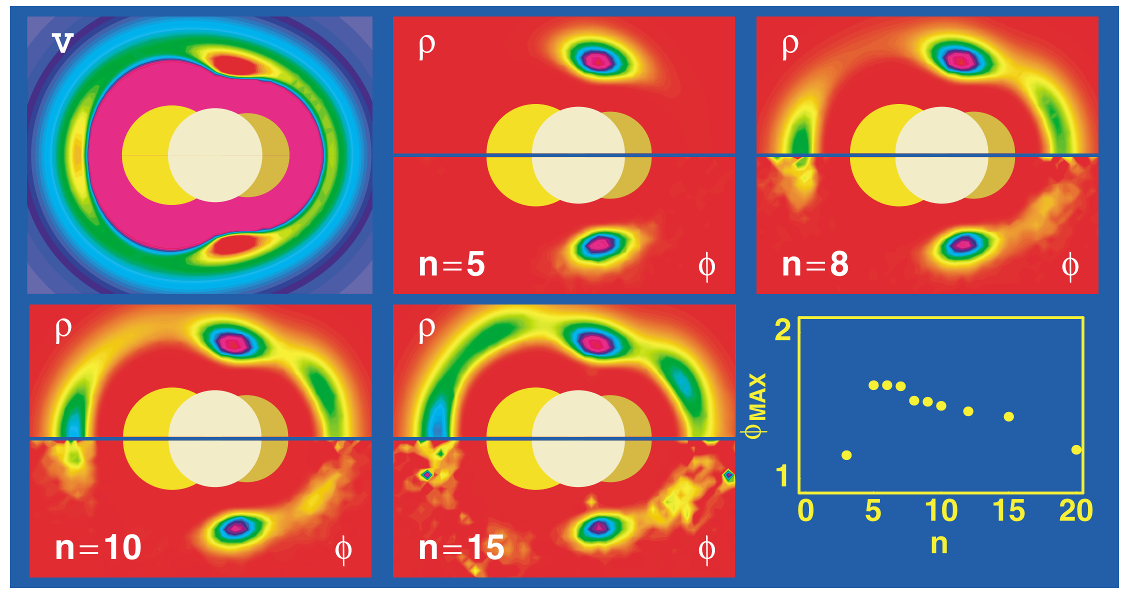
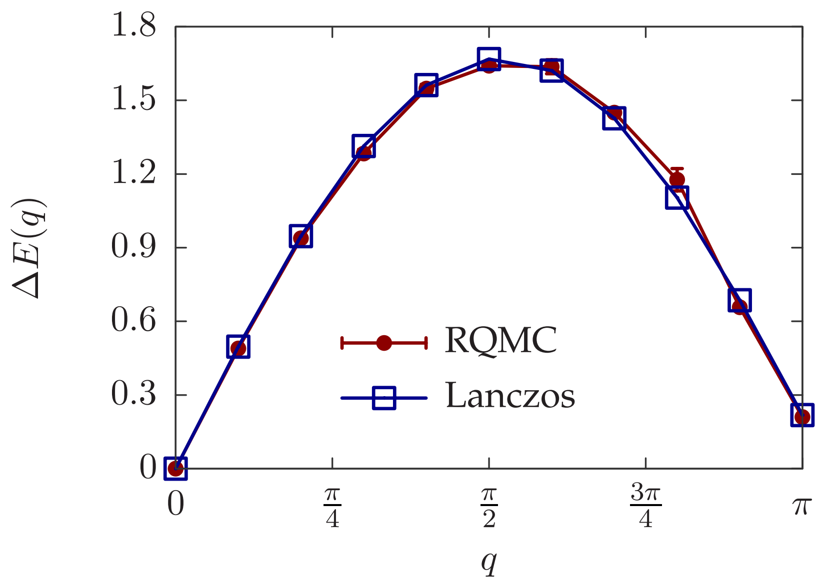


PHYSICAL REVIEW E **82**, 046710 (2010)

Reptation quantum Monte Carlo algorithm for lattice Hamiltonians with a directed-update scheme

Giuseppe Carleo, Federico Becca, Saverio Moroni, and Stefano Baroni



a few highlights

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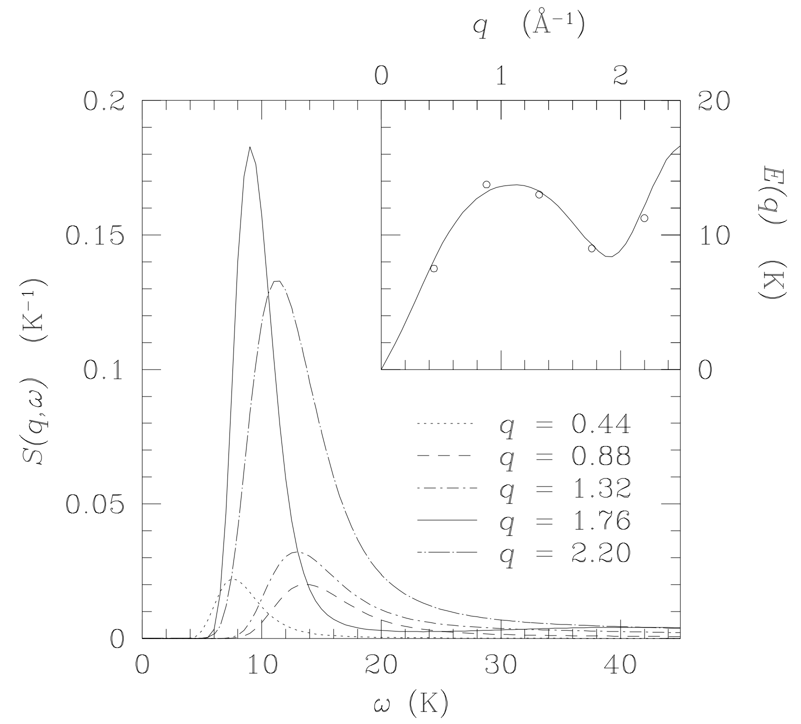

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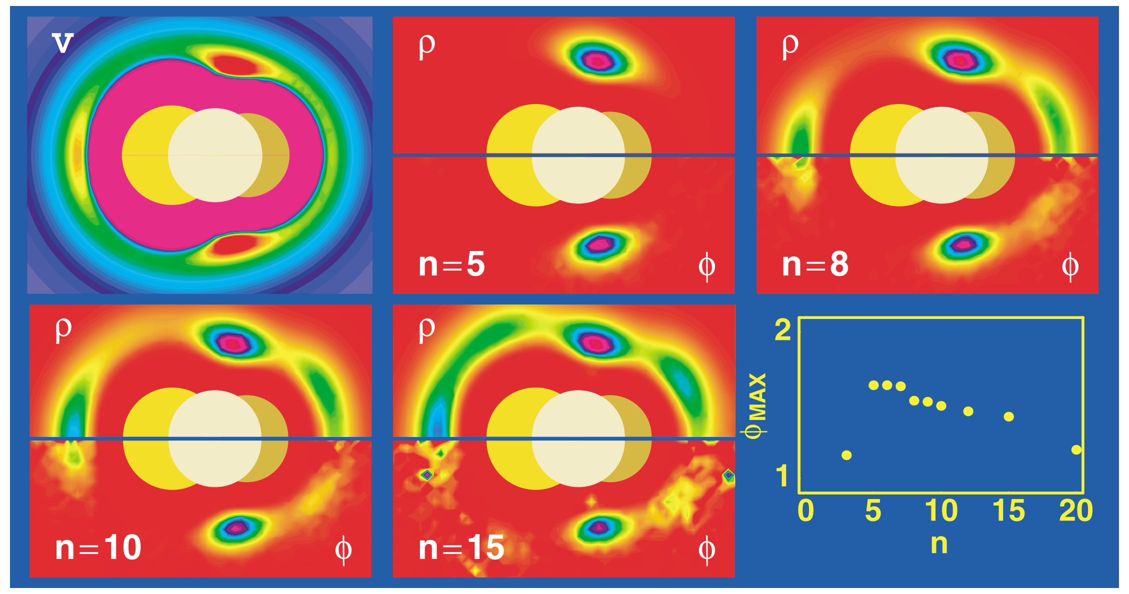

PHYSICAL REVIEW E **82**, 046710 (2010)

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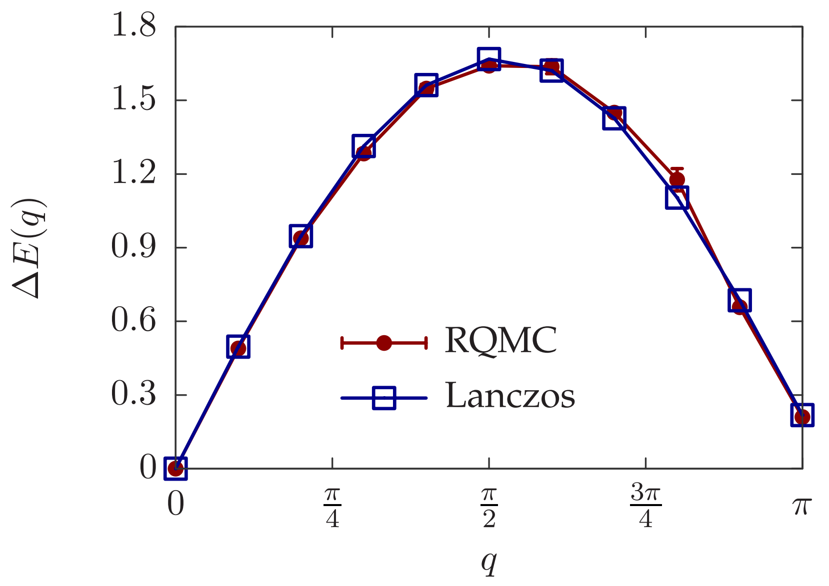
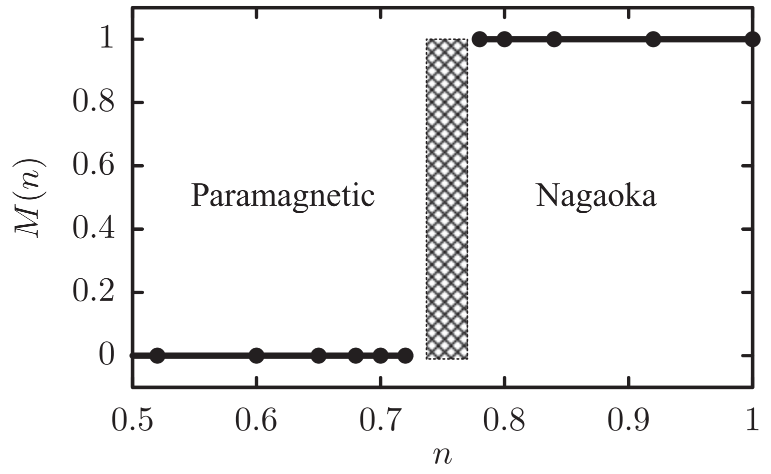


RAPID COMMUNICATIONS

PHYSICAL REVIEW B **83**, 060411(R) (2011)

Itinerant ferromagnetic phase of the Hubbard model

Giuseppe Carleo, Saverio Moroni, Federico Becca, and Stefano Baroni



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back to higher-order perturbation theory

$$\langle\Phi_0|e^{-\widehat{H}T}|\Phi_0\rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots$$

$$\log\langle\Phi_0|e^{-\widehat{H}T}|\Phi_0\rangle_{QM} = -\kappa_1 + \frac{1}{2}\kappa_2 + \cdots \frac{(-)^n}{n!}\kappa_n + \cdots$$

$$\begin{aligned}
\kappa_1 &= \mu_1 \\
\kappa_2 &= \mu_2 - {\mu_1}^2 && = \bar{\mu}_2 \\
\kappa_3 &= \mu_3 - 3\mu_2\mu_1 + 2{\mu_1}^3 && = \bar{\mu}_3 \\
\kappa_4 &= \mu_4 - 4\mu^3\mu_1 - \cdots && = \bar{\mu}_4 - 3\bar{\mu}_2^2 \\
&\cdots \\
\kappa_n &= \mu_n - \sum_{m=1}^{n-1}\binom{n-1}{m}\kappa_{n-m}\mu_m \\
&= \bar{\mu}_n - \sum_{m=1}^{n-2}\binom{n-1}{m}\kappa_{n-m}\bar{\mu}_m
\end{aligned}$$

$$\mu_n(T) = n!\int_0^T dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \langle\Phi_0|\widehat{\mathcal{W}}(t_n)\widehat{\mathcal{W}}(t_{n-1})\cdots\widehat{\mathcal{W}}(t_1)|\Phi_0\rangle_{QM}$$

back to higher-order perturbation theory

$$\langle\Phi_0|e^{-\widehat{H}T}|\Phi_0\rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots$$

$$\log\langle\Phi_0|e^{-\widehat{H}T}|\Phi_0\rangle_{QM} = -\kappa_1 + \frac{1}{2}\kappa_2 + \cdots \frac{(-)^n}{n!}\kappa_n + \cdots$$

$$\kappa_1 = \mu_1$$
$$\kappa_2 = \mu_2 - \mu_1{}^2 \qquad = \bar{\mu}_2$$
$$\kappa_3 = \mu_3 - 3\mu_2\mu_1 + 2\mu_1{}^3 \qquad = \bar{\mu}_3$$
$$\kappa_4 = \mu_4 - 4\mu^3\mu_1 - \cdots \qquad = \bar{\mu}_4 - 3\bar{\mu}_2^2$$
$$\cdots$$
$$\kappa_n = \mu_n - \sum_{m=1}^{n-1}\binom{n-1}{m}\kappa_{n-m}\mu_m$$
$$= \bar{\mu}_n - \sum_{m=1}^{n-2}\binom{n-1}{m}\kappa_{n-m}\bar{\mu}_m$$

$$\mu_n(T) = n!\int_0^T dt_n \int_0^{t_n} dt_{n-1}\cdots\int_0^{t_2} dt_1 \langle\Phi_0|\widehat{\mathcal{W}}(t_n)\widehat{\mathcal{W}}(t_{n-1})\cdots\widehat{\mathcal{W}}(t_1)|\Phi_0\rangle_{QM}$$

$$\begin{aligned} E_0 &= -\frac{d}{dT}\log\langle\Phi_0|e^{-\widehat{H}T}|\Phi_0\rangle \\ &= \dot{\kappa}_1 - \frac{1}{2}\dot{\kappa}_2 + \cdots \frac{1}{n!}\dot{\kappa}_n + \cdots \\ &= \not{\mathcal{E}_0} + E_0^{(1)} + E_0^{(2)} + \cdots E_0^{(n)} + \cdots \end{aligned}$$

back to higher-order perturbation theory

$$\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle_{QM} = 1 - \mu_1 + \frac{1}{2}\mu_2 + \cdots \frac{(-)^n}{n!}\mu_n + \cdots$$

$$\log\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle_{QM} = -\kappa_1 + \frac{1}{2}\kappa_2 + \cdots \frac{(-)^n}{n!}\kappa_n + \cdots$$

$$\begin{aligned}
\kappa_1 &= \mu_1 \\
\kappa_2 &= \mu_2 - {\mu_1}^2 && = \bar{\mu}_2 \\
\kappa_3 &= \mu_3 - 3\mu_2\mu_1 + 2{\mu_1}^3 && = \bar{\mu}_3 \\
\kappa_4 &= \mu_4 - 4\mu^3\mu_1 - \cdots && = \bar{\mu}_4 - 3\bar{\mu}_2^2 \\
&\cdots \\
\kappa_n &= \mu_n - \sum_{m=1}^{n-1}\binom{n-1}{m}\kappa_{n-m}\mu_m \\
&= \bar{\mu}_n - \sum_{m=1}^{n-2}\binom{n-1}{m}\kappa_{n-m}\bar{\mu}_m
\end{aligned}$$

$$\mu_n(T) = n!\int_0^T dt_n \int_0^{t_n} dt_{n-1}\cdots\int_0^{t_2} dt_1 \langle\Phi_0|\widehat{\mathcal{W}}(t_n)\widehat{\mathcal{W}}(t_{n-1})\cdots\widehat{\mathcal{W}}(t_1)|\Phi_0\rangle_{QM}$$

$$\begin{aligned}
E_0 &= -\frac{d}{dT}\log\langle\Phi_0|\mathrm{e}^{-\widehat{H}T}|\Phi_0\rangle \\
&= \dot{\kappa}_1 - \frac{1}{2}\dot{\kappa}_2 + \cdots \frac{1}{n!}\dot{\kappa}_n + \cdots \\
&= \not{\mathcal{E}}_0 + E_0^{(1)} + E_0^{(2)} + \cdots E_0^{(n)} + \cdots
\end{aligned}$$

$$E_0^{(n)} = \frac{(-)^{n+1}}{n!}\dot{\kappa}_n$$

back to higher-order perturbation theory

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$$\dot{\kappa}_n \sim \dot{\mu}_n^\circ - \sum_{m=1}^{n-1}\binom{n-1}{m}(\dot{\kappa}_{n-m}\mu_m^\circ + \kappa_{n-m}^\circ\dot{\mu}_m^\circ)$$

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$$= n!\sum_{k_1\cdots k_{n-1}} \mathcal{W}_{0k_1}\mathcal{W}_{k_1k_2}\cdots\mathcal{W}_{10}\int_0^T dt_n\int_0^{t_n} dt_{n-1}\cdots\int_0^{t_2} dt_1 \mathrm{e}^{-\mathcal{E}_{k_{n-1}}(t_n-t_{n-1})}\cdots\mathrm{e}^{-\mathcal{E}_{k_1}(t_2-t_1)}$$

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$$\mathcal{L}[\mu_n](z) = n!\sum_{k_1\cdots k_{n-1}}\frac{\mathcal{W}_{0k_1}\mathcal{W}_{k_1k_2}\cdots\mathcal{W}_{10}}{z^2(z+\mathcal{E}_{k_{n-1}})\cdots(z+\mathcal{E}_{k_1})}$$

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$$\mu_n^\circ \sim \text{zero-th order of } \frac{1}{(z+\mathcal{E}_1)\cdots(z+\mathcal{E}_n)} = \frac{1}{z^k(z+\mathcal{E}_1)\cdots(z+\mathcal{E}_{n-k})}$$

$$= \frac{1}{k!}\frac{d^k}{dz^k}\left(\frac{1}{(z+\mathcal{E}_1)\cdots(z+\mathcal{E}_{n-k})}\right)_{z=0} = \frac{1}{k!}\left(\frac{\partial}{\partial\mathcal{E}_1}+\frac{\partial}{\partial\mathcal{E}_{n-k}}\right)^k\frac{1}{\mathcal{E}_1\cdots\mathcal{E}_{n-k}}$$

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and similarly for $\dot{\mu}_0^n$

an example: third-order perturbation theory

$$E_0 = \dot{\kappa}_1 - \frac{1}{2}\dot{\kappa}_2 + \frac{1}{6}\dot{\kappa}_3 + \cdots$$

$$E_0^{(1)} \quad E_0^{(2)} \quad E_0^{(3)}$$

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$$\mathcal{L}[\dot{\mu}_3](z) = \frac{6}{z}\sum_{lm}\frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{(\mathcal{E}_l + z)(\mathcal{E}_m + z)}$$

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$$\kappa_3 = \mu_3 - 3\mu_2\mu_1 + 2\mu_1^2$$

$$\begin{aligned}\dot\kappa_3 &= \dot\mu_3 - 3\dot\mu_2\mu_1 + 3\mu_2\dot\mu_1 + 6\dot\mu_1\mu_1^2 \\ &\sim \dot\mu_3^\circ + 3\mu_2^\circ\dot\mu_1\end{aligned}$$

$$\begin{aligned}\mathcal{L}[\dot\mu_3](z) &= \frac{6}{z}\sum_{lm}\frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{(\mathcal{E}_l+z)(\mathcal{E}_m+z)} \\ &= \frac{6}{z}\sum_{lm}{}'\frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{(\mathcal{E}_l+z)(\mathcal{E}_m+z)} + \frac{12\mathcal{W}_{00}}{z}\sum_{l}{}'\frac{\mathcal{W}_{l0}^2}{(\mathcal{E}_l+z)} \\ &= \frac{1}{z}6\left[\sum_{lm}{}'\frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{\mathcal{E}_l\mathcal{E}_m} - 2\mathcal{W}_{00}\sum_{l}{}'\frac{\mathcal{W}_{l0}^2}{\mathcal{E}_l^2}\right] + \mathcal{O}\left(z^{-2}\right)\end{aligned}$$

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$$\begin{aligned}
\mathcal{L}[\dot{\mu}_3](z) &= \frac{6}{z}\sum_{lm}\frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{(\mathcal{E}_l+z)(\mathcal{E}_m+z)} \\
&= \frac{6}{z}\sum_{lm}{}' \frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{(\mathcal{E}_l+z)(\mathcal{E}_m+z)} + \frac{12\mathcal{W}_{00}}{z}\sum_{l}{}' \frac{\mathcal{W}_{l0}^2}{(\mathcal{E}_l+z)} \\
&= \frac{1}{z}6\left[\sum_{lm}{}' \frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{\mathcal{E}_l\mathcal{E}_m} - 2\mathcal{W}_{00}\sum_{l}{}' \frac{\mathcal{W}_{l0}^2}{\mathcal{E}_l^2}\right] + \mathcal{O}\left(z^{-2}\right)
\end{aligned}$$

$$\mathcal{L}[\mu_2](z) = \frac{2}{z^2}\sum_l \frac{\mathcal{W}_{0l}^2}{\mathcal{E}_l + z}$$

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$$= \frac{6}{z}{\sum_{lm}}'\frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{(\mathcal{E}_l + z)(\mathcal{E}_m + z)} + \frac{12\mathcal{W}_{00}}{z}{\sum_{l}}'\frac{\mathcal{W}_{l0}^2}{(\mathcal{E}_l + z)}$$
$$= \frac{1}{z}6\left[{\sum_{lm}}'\frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{\mathcal{E}_l\mathcal{E}_m} - 2\mathcal{W}_{00}{\sum_{l}}'\frac{\mathcal{W}_{l0}^2}{\mathcal{E}_l^2}\right] + \mathcal{O}\left(z^{-2}\right)$$

$$\mathcal{L}[\mu_2](z) = \frac{2}{z^2}\sum_{l}\frac{\mathcal{W}_{0l}^2}{\mathcal{E}_l + z}$$
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$$= \frac{1}{z}6\left[\sum_{lm}{}'\frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{\mathcal{E}_l\mathcal{E}_m} - 2\mathcal{W}_{00}\sum_{l}{}'\frac{\mathcal{W}_{l0}^2}{\mathcal{E}_l^2}\right] + \mathcal{O}\left(z^{-2}\right)$$

$$E_0^{(3)} = \sum_{lm}{}'\frac{\mathcal{W}_{0l}\mathcal{W}_{lm}\mathcal{W}_{m0}}{\mathcal{E}_l\mathcal{E}_m} - \mathcal{W}_{00}\sum_{l}{}'\frac{\mathcal{W}_{l0}^2}{\mathcal{E}_l^2}$$

$$\mathcal{L}[\mu_2](z) = \frac{2}{z^2}\sum_{l}\frac{\mathcal{W}_{0l}^2}{\mathcal{E}_l+z}$$

$$= \frac{1}{z}\left[-2\sum_{l}{}'\frac{\mathcal{W}_{l0}^2}{\mathcal{E}_l^2}\right] + \mathcal{O}\left(z^{-2}\right)$$


keep dreaming and flying high for another 60 years, dude!

thanks

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- to all of you, for bearing with me today

these slides available soon at https://talks.baroni.me