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Long-Range Random Walks on Energetically Disordered Lattices

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Although the master equation describing long-range random walks on an energetically disordered lattice is governed by a nonsymmetric transition matrix W, it may be mapped through a similarity transform onto an imaginary-time Schrödinger equation governed by a Hermitian (Hamiltonian) operator H_0 having a nondegenerate ground state. Under this mapping the diffusion constant D can be expressed in terms of the exact ground state energy of operators that are infinitesimally perturbed from H_0.

Historically, the similarities between the diffusion equation and the Schrödinger equation have been profitably exploited by workers interested in both [1,2]. It is well known, for example, that the master equation describing a *symmetric* lattice random walk (by which we mean one in which the hopping rate between two sites is the same going both forwards and backwards) is isomorphic to an imaginary-time Schrödinger equation evolving under a one particle tight-binding Hamiltonian. The symmetry of the hopping rates between forward and backward jumps is reflected in the Hermiticity of the corresponding lattice Hamiltonian. What is not often appreciated, however, is that under most physically relevant conditions even a *nonsymmetric* random walk (describing, for example, hopping diffusion in an *energetically disordered* system) may be mapped through a similarity transform onto a quantum system evolving according to an imaginary time Schrödinger equation [2]. The lattice Hamiltonian H_0 which governs this evolution is Hermitian and possesses an easily calculable, nondegenerate ground state. In this Letter we present details of this transformation and use it to derive an exact spectral representation for the diffusion constant D. We also show how the diffusion constant can be expressed in terms of the exact ground state energy of operators infinitesimally perturbed from H_0. This observation leads to a new and useful method for calculating the diffusion constant for such systems. As an application of the approach we derive in a simple way exact results for the long-range symmetric random well problem [3].

A long-range random walk on an energetically disordered d-dimensional lattice can be described through the master equation

$$\frac{dP_s}{dt} = \sum_{s'}(F_{s,s'}P_{s'} - F_{s',s}P_s) , \qquad (1)$$

in which $P_s(t)$ describes the probability of finding the particle at the site of lattice vector $s = (s_1, \ldots, s_d)$ at time t. The hopping rate $F_{s,s'} = F(|s - s'|; \varepsilon_s, \varepsilon_{s'})$ from site s' to s is assumed to depend upon the distance $|s - s'|$ and upon the randomly and independently distributed energies ε_s and $\varepsilon_{s'}$ of the two sites involved in the transition. Because of this energy difference, the rates connecting two sites are not generally symmetric; i.e., forward and backward hopping rates are not generally equal. In most

systems of physical interest, however, a detailed balance relation [4] of the form $F_{s,s'}\rho(\varepsilon_{s'}) = F_{s',s}\rho(\varepsilon_s)$ relates forward and backward hopping rates to one another through the relative equilibrium probability $\rho(\varepsilon)$ of finding the particle at a site of energy ε. Indeed, in most cases the equilibrium distribution associated with the system is unique and known *a priori* based upon the statistics (for example, Boltzmann or Fermi-Dirac) of the transport particles of interest. We assume this to be the case in what follows, although we will not need to specify the precise functional form of the distribution.

To proceed, it is convenient to consider an infinite lattice that is periodically extended from the original (finite but large) energetically disordered crystal in all directions. This new system is infinite in extent and invariant under translations T_L along crystal axes by multiples of the edge length L of the crystal (assumed cubic), with each superunit cell (or supercell) containing an identical random array of $N = L^d$ sites (unit lattice spacing is assumed throughout). Corresponding sites in each cell have the same energy, i.e., $\varepsilon_s = \varepsilon_{s+L}$. The distance and energy dependence of hopping rates in the new infinitely replicated system are assumed to be functionally identical to those in the original crystal. This leads to equations of motion for the periodically repeated crystal

$$\frac{dP_s^n}{dt} - \sum_{m,s'} W_{ss'}^{n-m} P_s^m = 0 , \qquad (2)$$

in which P_s^n denotes the probability for the particle to be at lattice vector $r_s^n = n + s$ of the infinite system, and $W_{ss'}^m = F_{ss'}^m - \delta_{m,0}\delta_{s,s'}\Omega_s$. In these expressions the superlattice vector (or supercell index) $n = (n_1, \ldots n_d)L$ locates the origin of the corresponding supercell, the intracell position vectors $s = (s_1, \ldots s_d)$ locate sites within each supercell, and we have defined $\Omega_s = \sum_{m,s'} F_{s's}^m$. Translational invariance on length scale L implies that the hopping rate connecting sites in different supercells $F_{ss'}^{mn} = F(|m + s - n - s'|; \varepsilon_s, \varepsilon_{s'}) = F_{ss'}^{m-n}$ depends upon the supercell indices m and n only through the net displacement vector $m - n$ connecting them. Note that these rates connect sites within a single cell ($m - n = 0$), as well as sites in cells separated by an arbitrarily large superlattice vector. Thus, no truncation of long-range effects will occur, despite the finite supercell size. The detailed balance condition in the repeated system can now be expressed,

$W_{s's}^m \rho_s^0 = W_{ss'}^{-m} \rho_{s'}^0$, in terms of equilibrium populations $\rho_s^0 = \lim_{t \to \infty} \sum_n P_s^n(t) = \rho(\varepsilon_s)/\sum_{s'} \rho(\varepsilon_{s'})$ normalized to one particle. Again, these populations are assumed to be known or calculable from the density of states, temperature, etc.

The detailed balance relation implies that the transition matrix W is generally not symmetric except when all sites are degenerate. As we have suggested, however, it is possible to introduce a similarity transformation to a set of variables governed by a Hermitian transition matrix [2,4]. We introduce the (directly calculable) quantities $\phi_s^0 = (\rho_s^0)^{1/2}$, which we use to define similarity transforms $\Psi_s^n(t) \equiv (1/\phi_s^0) P_s^n(t)$ of the probabilities and of the transition matrix

$$H_{ss'}^{mn} \equiv (1/\phi_s^0) W_{ss'}^{m-n} \phi_{s'}^0 = (1/\phi_s^0)(W_{s's}^{n-m} \rho_s^0/\rho_{s'}^0) \phi_{s'}^0$$
$$= (1/\phi_{s'}^0) W_{s's}^{n-m} \phi_s^0 = H_{s's}^{nm} .$$

Applying this to (2) yields an "imaginary-time" Schrödinger equation,

$$\frac{d\Psi_s^n}{dt} - \sum_{m,s'} H_{ss'}^{n-m} \Psi_{s'}^m = 0 \qquad (3)$$

governed now by a Hamiltonian matrix $H_{ss'}^m = H_{s's}^{-m}$ which is Hermitian (in fact, real symmetric) and which therefore possesses a complete orthonormal set of eigenvectors. The Laplace transform of (3) is

$$\varepsilon \psi_s^n - \sum_{m,s'} H_{ss'}^{n-m} \psi_{s'}^m = \Psi_s^n(0) , \qquad (4)$$

in which $\psi_s^n(\varepsilon)$ is the Laplace transform at "energy" (frequency) ε of the "wave" function $\Psi_s^n(t)$. The initial condition of interest $P_s^n(0) = \delta_{n,0} \delta_{s,0}$, corresponding to one particle placed initially at the origin, has as its similarity transform the expression $\Psi_s^n(0) = (1/\phi_0^0) \delta_{n,0} \delta_{s,0}$. We now introduce a spatial Fourier transform $\psi_s^k(\varepsilon) = \sum_n e^{-i\mathbf{k} \cdot (\mathbf{n}+\mathbf{s})} \psi_s^n(\varepsilon)$ over the supercell index $\mathbf{n}$, obtaining

$$\varepsilon \psi_s^k - \sum_{s'} H_{ss'}^k \psi_{s'}^k = \Psi_s^k(0) = \Psi_s(0) , \qquad (5)$$

in which $\Psi_s^k(0) = \Psi_s(0) = (1/\phi_0^0) \delta_{s,0}$ is, as our notation suggests, independent of k. Introducing Dirac notation we identify (5) as the projection onto site state $|s\rangle$ of the equation

$$(\varepsilon - H_k)|\psi^k\rangle = |\Psi_0\rangle , \qquad (6)$$

in which H_k is the $N \times N$ matrix with elements $H_{ss'}^k \equiv \sum_m e^{-i\mathbf{k} \cdot (\mathbf{m}+\mathbf{s}-\mathbf{s}')} H_{ss'}^m$, and the N-dimensional vectors $|\psi^k\rangle = |\psi^k(\varepsilon)\rangle$ and $|\Psi_0\rangle$ have components $\psi_s^k(\varepsilon)$ and $\Psi_s(0)$, respectively. This equation admits the formal solution $|\psi^k\rangle = G^k(\varepsilon)|\Psi_0\rangle$, where $G^k(\varepsilon) = (\varepsilon - H_k)^{-1}$ is the Green's function or resolvent matrix associated with the Hamiltonian H_k. A few features of this formal solution are all that we use. We observe, first, that the small-k, small-ε limit of the components of the column vector $|\psi^k\rangle$ are directly related to the equilibrium quantities ϕ_s^0 which generate the similarity transformation. Using a Tauberian theorem, along with the definition of $\Psi_s^n(t)$, it follows that

$$\lim_{\substack{k \to 0 \\ \varepsilon \to 0}} \varepsilon \psi_s^k = \lim_{\varepsilon \to 0} \sum_n \varepsilon \psi_s^n = \lim_{t \to \infty} \sum_n \Psi_s^n(t) = \phi_s^0 , \qquad (7)$$

where the ϕ_s^0 are (through their definition) square normalized to unity. Indeed, the normalized state vector $|\phi_0\rangle \equiv \lim_{k,\varepsilon \to 0} \varepsilon |\psi^k(\varepsilon)\rangle$ with components ϕ_s^0 is the (unique) eigenvector corresponding to the zero energy eigenvalue of the ($k = 0$) Hamiltonian $H_0 = \lim_{k \to 0} H_k$. To see this, multiply (6) by ε and take the limit

$$\lim_{\substack{k \to 0 \\ \varepsilon \to 0}} (\varepsilon - H_k)\varepsilon |\psi^k(\varepsilon)\rangle = \lim_{\varepsilon \to 0} \varepsilon |\Psi_0\rangle = 0 ,$$

which implies that $H_0 |\phi_0\rangle = 0$. The vector $|\phi_0\rangle$ therefore plays the role of the "ground state" for the Hermitian operator H_0. (It is actually the ground state of the positive operator $-H_0$, a distinction which has no consequence to what follows [5].) Note that it is the assumed uniqueness of the equilibrium distribution which implies the nondegeneracy of the ground state of this effective Hamiltonian.

The mapping of the nonsymmetric diffusion problem onto this related quantum system, while of some formal interest, would be of limited utility if it did not lead to new results or simpler expressions for calculating relevant quantities such as transport coefficients. In what follows we use this mapping to derive new expressions for the diffusion constant D, which characterizes the linear asymptotic growth of the mean squared displacement for a particle initially localized at the origin. In the periodically extended lattice, this can be written

$$2dD = \lim_{t \to \infty} \frac{d}{dt} \sum_{\mathbf{n},s} (\mathbf{n}+\mathbf{s})^2 P_s^n(t) . \qquad (8)$$

The diffusion constant may be obtained from the small-k, small-ε limit of $\psi_s^k(\varepsilon)$. Through the similarity transformation already defined and a Tauberian theorem we find

$$2dD = \lim_{t \to \infty} \frac{d}{dt} \sum_{\mathbf{n},s} (\mathbf{n}+\mathbf{s})^2 \phi_s^0 \Psi_s^n(t)$$
$$= -\lim_{\substack{k \to 0 \\ \varepsilon \to 0}} \sum_s \phi_s^0 \varepsilon^2 \nabla_k^2 \psi_s^k(\varepsilon)$$
$$= -\lim_{\substack{k \to 0 \\ \varepsilon \to 0}} \sum_{s,s'} \phi_s^0 [\varepsilon^2 \nabla_k^2 G_{s,s'}^k(\varepsilon)] \Psi_{s'}(0)$$
$$= -\lim_{\substack{k \to 0 \\ \varepsilon \to 0}} \langle \phi_0 | \varepsilon^2 \nabla_k^2 G^k(\varepsilon) | \Psi_0 \rangle . \qquad (9)$$

It is convenient to transfer the derivatives of the operator $G^k(\varepsilon)$ appearing in (9) to those of the operator H_k. Using the compact notation $G = G^k$, $H = H_k$, we note that $GG^{-1} = 1$. Thus,

$$\nabla_k \{GG^{-1}\} = 0 = \{\nabla_k G\} G^{-1} + G\{\nabla_k (G^{-1})\} .$$

Since $\nabla_k(G^{-1}) = -\nabla_k H$, this implies that

$$\nabla_k G = G(\nabla_k H)G .$$

It is then a straightforward extension to show that $\nabla_k^2 G = G[\nabla_k^2 H - 2(\nabla_k H) \cdot G(\nabla_k H)]G$. This allows us to

pass to the zero wave-vector limit. We define for nonzero ε the $k=0$ limits; $g(\varepsilon) \equiv \lim_{k \to 0} G^k; V_0 = \lim_{k \to 0} -V_k^2 H_k$; and the vector operator $V \equiv \lim_{k \to 0}(-\nabla_k H_k)$. The diffusion constant (9) can then be written $2dD = \lim_{\varepsilon \to 0} \langle \phi_0 | \varepsilon g \{V_0 - 2V \cdot gV\} \varepsilon g | \Psi_0 \rangle$. To put this in a more convenient form, the operator $g = (\varepsilon - H_0)^{-1}$ can be expanded in the orthonormal basis $\{|\phi_\lambda\rangle\}$ of eigenvectors of H_0; i.e., we can write

$$g(\varepsilon) = \frac{|\phi_0\rangle\langle\phi_0|}{\varepsilon} + \sum_{\lambda \neq 0} \frac{|\phi_\lambda\rangle\langle\phi_\lambda|}{\varepsilon - \varepsilon_\lambda} , \qquad (10)$$

where we have again used the uniqueness of the equilibrium configuration to explicitly separate out the zero eigenvector. It is apparent that the operator $\lim_{\varepsilon \to 0} \varepsilon g(\varepsilon) = |\phi_0\rangle\langle\phi_0|$ is the projector onto the ground (i.e., equilibrium) state. Using this result and the fact that $\langle\phi_0|\Psi_0\rangle = \sum_s (\phi_s^0/\phi_s^0)\delta_{s,0} = 1$, we can express the diffusion constant as a ground state expectation value

$$D = (1/2d)\lim_{\varepsilon \to 0} \langle\phi_0|\{V_0 - 2V \cdot gV\}|\phi_0\rangle = \langle\phi_0|\hat{D}|\phi_0\rangle \qquad (11)$$

of the operator $\hat{D} = \lim_{\varepsilon \to 0}\{V_0 - 2V \cdot gV\}/2d$. The second part of this diffusion operator $\hat{D}$ contains information about fluctuations induced in the ground state by the operator V. To see this we use (10) to write

$$\langle\phi_0|V \cdot g(\varepsilon)V|\phi_0\rangle = \sum_{\lambda,\alpha} \frac{\langle\phi_0|V_\alpha|\phi_\lambda\rangle\langle\phi_\lambda|V_\alpha|\phi_0\rangle}{\varepsilon - \varepsilon_\lambda} , \qquad (12)$$

where V_α, with $\alpha = 1, \ldots, d$, represents the Cartesian components of $V \equiv \lim_{k \to 0}(-\nabla_k H_k)$. It follows from the

definition and symmetry of H_k that the operator V is both antisymmetric and strictly imaginary in the site representation, i.e.,

$$\langle s|V|s'\rangle = i\sum_m (m+s-s')H_{ss'}^m = i\sum_m (m+s-s')H_{s's}^{-m}$$
$$= -i\sum_m (m+s'-s)H_{s's}^m = -\langle s'|V|s\rangle . \qquad (13)$$

Thus V is also Hermitian. The reality of the components ϕ_s^0 of $|\phi_0\rangle$ can then be used to show that the ground state expectation value of V vanishes, i.e.,

$$\langle\phi_0|V|\phi_0\rangle = \sum_{s,s'} \phi_s^0\langle s'|V|s\rangle\phi_s^0 = -\sum_{s,s'} \phi_s^0\langle s|V|s'\rangle\phi_s^0$$
$$= -\sum_{s,s'} \phi_s^0\langle s|V|s'\rangle\phi_{s'}^0 = -\langle\phi_0|V|\phi_0\rangle . \qquad (14)$$

Thus, the $\lambda = 0$ term in (12) can be omitted, allowing us to take the zero frequency limit without worrying about singularities:

$$\lim_{\varepsilon \to 0} \langle\phi_0|V \cdot g(\varepsilon)V|\phi_0\rangle = -\sum_{\lambda \neq 0,\alpha} \frac{|\langle\phi_0|V_\alpha|\phi_\lambda\rangle|^2}{\varepsilon_\lambda} . \qquad (15)$$

This leads to the following *exact* spectral representation of the diffusion constant in the eigenstates of H_0:

$$2dD = \langle\phi_0|V_0|\phi_0\rangle + 2\sum_{\lambda \neq 0,\alpha} \frac{|\langle\phi_0|V_\alpha|\phi_\lambda\rangle|^2}{\varepsilon_\lambda - \varepsilon_0} . \qquad (16)$$

The first term on the right-hand side of (16) is readily calculable in terms of the known ground state $|\phi_0\rangle$. From the definitions appearing above it follows that

$$D_0 \equiv \langle\phi_0|V_0|\phi_0\rangle = \sum_{s,s'} \phi_s^0\langle s'|V_0|s\rangle\phi_{s'}^0 = \sum_{m,s,s'} (m+s'-s)^2 \phi_s^0 H_{s's}^m \phi_s^0$$
$$= \sum_{m,s,s'} (m+s'-s)^2 W_{s's}^m \phi_s^0 \phi_s^0 = \sum_{m,s,s'} (m+s'-s)^2 F(|m+s'-s|;\varepsilon_{s'},\varepsilon_s)\rho_s^0 . \qquad (17)$$

In the last line, we may replace the sum over m and s' with a sum over all lattice vectors $r = m + s'$, and set $\varepsilon_r = \varepsilon_{s'}$ to obtain the simple result

$$D_0 = \frac{1}{2d}\sum_{r,s} |r-s|^2 F(|r-s|;\varepsilon_r,\varepsilon_s)\rho_s^0 , \qquad (18)$$

the form of which remains invariant in the thermodynamic limit $(L \to \infty)$. The second term on the right-hand side of (16) is not so trivial. We have included the superfluous value $\varepsilon_0 = 0$ in the denominator to emphasize the structure of this term, which (although exact) is a sum of terms having precisely the *form* of the second order energy shift [6] induced by a small perturbation in the ground state energy of the unperturbed Hamiltonian H_0. Of course the perturbing operators $H^\alpha = \sqrt{2}V_\alpha$ implied by this expression are not generally small compared to H_0. Consider, however, the family of operators $H_\alpha(\eta) = H_0 + \eta H^\alpha$ that are *infinitesimally* close to H_0. We know from perturbation theory that since [as shown by (14)] the operator H^α has zero expectation value with respect to the unperturbed ground state $|\phi_0\rangle$, the first order corrections to the perturbed ground state energy (i.e., corrections linear in η) will vanish. The lowest nonvan-

ishing correction to the ground state energy will therefore be second order in η. Since the unperturbed ground state energy itself vanishes, this implies that the *exact* ground state energy $\varepsilon_0^\alpha(\eta)$ of the Hamiltonian $H_\alpha(\eta)$ will vanish as η^2 for infinitesimal η, and that the second term appearing in (16) will be the coefficient of this η^2 term. We thus make the identification

$$D_\alpha \equiv 2\sum_\lambda \frac{|\langle\phi_0|V_\alpha|\phi_\lambda\rangle|^2}{\varepsilon_\lambda - \varepsilon_0} = \lim_{\eta \to 0} [\eta^{-2}\varepsilon_0^\alpha(\eta)] . \qquad (19)$$

Equations (16)-(19) are the main formal results of this Letter. These expressions may be used both analytically and computationally to investigate the transport properties of energetically disordered systems. They allow us, for example, to derive in a simple way the exact diffusion constant for the long-range *symmetric well* problem [3]. In this model, the hopping rate between two sites is allowed to depend upon the distance between the two sites and upon the energy of the site (or well) from which a particular hop occurs, but is *independent* of the energy of the site to which the particle is hopping. The physical picture behind this model is that of a set of wells of random depth separated by tall barriers of uniform

height. Thus, after obtaining the energy to leave the initial well, the particle is able, in principle, to make jumps to any other site in the crystal with a hopping probability that depends only upon the distance. This is a natural extension of the nearest-neighbor symmetric well problem treated elsewhere [3]. Under these conditions, the hopping rates can be written in the simplified form $F_{s,s'}$

$= F(|s - s'|; \varepsilon_{s'})$. We wish to show that in this limit the second term in (16) vanishes, so that the entire diffusion constant is contained in the easily calculable first term (18). A close inspection of (16) reveals that this second term will vanish if the quantity $\langle \phi_\lambda | V | \phi_0 \rangle = \sum_s \langle \phi_\lambda | s \rangle \times \langle s | V | \phi_0 \rangle$ is equal to zero. To demonstrate this we evaluate the factor

$$\langle s | V | \phi_0 \rangle = \sum_{s'} \langle s | V | s' \rangle \phi_{s'}^0 = i \sum_{m,s'} (\mathbf{m} + \mathbf{s} - \mathbf{s}') H_{ss'}^m \phi_{s'}^0$$

$$= i \sum_{m,s'} (\mathbf{m} + \mathbf{s} - \mathbf{s}') H_{s's}^{-m} \phi_{s'}^0 = -i \sum_{m,s'} (\mathbf{m} + \mathbf{s}' - \mathbf{s}) [(1/\phi_{s'}^0) W_{s's}^m \phi_s^0] \phi_{s'}^0$$

$$= -i \phi_s^0 \sum_{m,s'} (\mathbf{m} + \mathbf{s}' - \mathbf{s}) F(|\mathbf{m} + \mathbf{s}' - \mathbf{s}|; \varepsilon_s) = -i \phi_s^0 \sum_r \mathbf{r} F(|\mathbf{r}|; \varepsilon_s) . \tag{20}$$

In the last line, we have replaced the sum over $\mathbf{m}$ and $\mathbf{s}'$ with a sum over all lattice vectors $\mathbf{r} = \mathbf{m} + \mathbf{s}'$, and shifted the origin to the site s. However, the last sum is clearly zero for a centrosymmetric lattice, since the summand is an odd function of the lattice vector $\mathbf{r}$. It follows that the diffusion constant for the long-range symmetric well problem on a centrosymmetric lattice is given by the first term in (16), which reduces in this limit to

$$D_0 = \frac{1}{2d} \sum_{r,s} |\mathbf{r}|^2 F(|\mathbf{r}|; \varepsilon_s) \rho(\varepsilon_s) . \tag{21}$$

The general expression (16) also lends itself to a number of computational schemes for computing the diffusion constant for energetically disordered lattices which we sketch below. The first is a straightforward implementation of (16): A large cubic region of the crystal containing a random distribution of site energies is generated in the computer and its transition matrix is determined. The corresponding Hamiltonian is constructed, and diagonalized numerically. The resulting eigenvalues and eigenvectors are then used to evaluate the diffusion constant directly through (17).

A second scheme which we have implemented exploits the observed relationship of the diffusion constant to perturbation theoretical expressions, such as (17). Thus we search for the ground state energy $\varepsilon_0^g(\eta)$ of $H_\alpha(\eta)$, writing the infinitesimally perturbed ground state in the form $|\phi_0(\eta)\rangle = |\phi_0\rangle + \eta|\delta\rangle$, where the vector $|\delta\rangle$ can be assumed orthogonal to the unperturbed ground state $|\phi_0\rangle$. From (19) the ground state energy itself can be written in the form $\varepsilon_0^g(\eta) = \eta^2 D_\alpha$. Substituting these expressions into the eigenvalue equation $H_\alpha(\eta)|\phi_0(\eta)\rangle = \varepsilon_0^g(\eta)|\phi_0(\eta)\rangle$ and equating coefficients of corresponding powers of η we find that $H_\alpha|\phi_0\rangle = -H_0|\delta\rangle$, and $D_\alpha|\phi_0\rangle = H_\alpha|\delta\rangle$. This latter relation allows the quantity of interest $D_\alpha = \langle\phi_0|H_\alpha|\delta\rangle$ to be calculated once the vector $|\delta\rangle$ is obtained. Since $|\phi_0\rangle$ and H_α are known, $|\delta\rangle$ can be evaluated from the first of the two relations expressed above as the solution to the equation $H_0|\delta\rangle = |f\rangle$, where $|f\rangle = H_\alpha|\phi_0\rangle$. A comparative report dealing with both of these numerical procedures will be reported in a later publication. As a final point we note that since the diffusion constant can be expressed in

terms of the exact ground state energy of well-defined operators this approach naturally lends itself to the development of variational bounds which involve the (analytical or numerical) minimization of the mean energy for a suitable family of trial vectors.

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